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Octree Bin-to-Bin Fractional-NTC Collisions

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Air Force Research Laboratory
Edwards Air Force Base, CA USA

DSMC 2015

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Outline

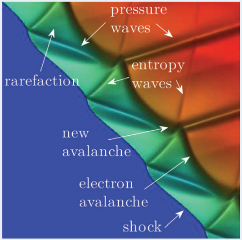
Important Collisions in Spacecraft Propulsion:

- Discharge and Breakdown in FRC
- Collisional Radiative Cooling/Ionization
- Combustion Chemistry

Common Features in Spacecraft Collisions:

- Relevant Densities Spanning Many Orders of Magnitude — 6+
- Transitions from Collisional to Collisionless
- Tiny Early e^- or Radical Populations Critical to Induction Delay
- Many types of Inelastic Collisions with Unknown Effects on Distribution Shapes

Shock Ionization



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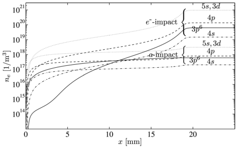

Importance of Collision Physics

Important Collisions in Spacecraft Propulsion:

- Discharge and Breakdown in FRC
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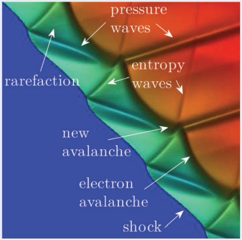
Need Low Noise & High Dynamic Range Collision Algorithms

Shock Ionization



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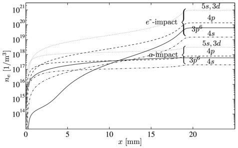


Standard Collision Models

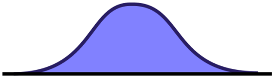
<u>Previous Collision Methods:</u>

- Monte Carlo Collisions (MCC)
  - Particles Collide with Background "Fluid"
  - Often Used in Plasma/PIC Simulation
  - Ion-e^- Collisions Assume Stationary Ions
  - No Conservation/Detailed Balance
- Direct Simulation Monte Carlo Collisions (DSMC)
  - Most Modern Versions use No-Time Counter (NTC) Method
  - Conservative/Reversible Collision
  - Satisfies Detailed Balance
  - Subset of Possible Collisions Sampled
  - Random Selection vs Z_{ij} for All/Nothing Collision

All Random Flip vs Number of Collisions: $Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle \, \mathrm{dt}$

Continuum to Discrete Representation:

- Many Particles $\rightrightarrows$ Continuous Distribution



Variable Weights for Dynamic Range

Continuum to Discrete Representation:

- Many Particles $\rightsquigarrow$ Continuous Distribution
- Discretized VDF Yields Vlasov
  But Collision Integral Still a Problem

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- Collisions between Discrete Velocities

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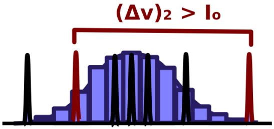

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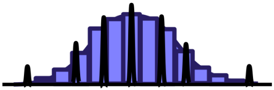

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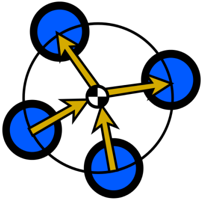
Variable Weight “All-or-Nothing” Collisions?



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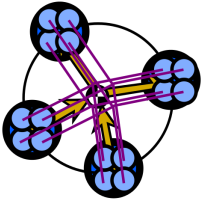

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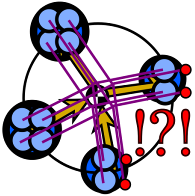
Variable Weight "All-or-Nothing" Collisions?
Physically Inconsistent!
(Mixing Violates Momentum/Energy Conservation)



NTC Collisions:

- (Collision Rate Volume):(Cell Volume)

Fractional-NTC Collisions:

$$Z_{ij} = \frac{n_i n_j}{2} \left\langle \sigma v \right\rangle_{ij} \mathrm{dt} = \frac{w_i w_j}{2V_{cell}^2} \left\langle \sigma v \right\rangle_{ij} \mathrm{dt}$$

NTC Collisions:

- (Collision Rate Volume):(Cell Volume)
- Select Fraction of $\frac{1}{2}N^2$ Possible

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$$P_{ij} = w \langle \sigma v \rangle_{ij} \, \mathrm{dt}/V_{cell}$$
$$P_{max} = w \langle \sigma v \rangle_{ij}^{max} \, \mathrm{dt}/V_{cell}$$
$$N_{select} = \frac{N_p^2}{2} F_n \langle \sigma v \rangle_{ij}^{max} \, \mathrm{dt}/V_{cell}$$

Fractional-NTC Collisions:

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Collide if:

$$\mathtt{Rand(1)} < \frac{N_{collide}}{N_{select}} = \frac{P_{ij}}{P_{max}} = \frac{\langle \sigma v \rangle_{ij}}{\langle \sigma v \rangle_{ij}^{max}}$$

NTC Collisions:

- (Collision Rate Volume):(Cell Volume)
- Select Fraction of $\frac{1}{2}N^2$ Possible
- Probability of Event Ratio of Volumes
- Correct Non-Equilibrium Frequency

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Fractional-NTC Collisions:

- Select f by Cost/Accuracy Tradeoff

$$Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle_{ij} \mathrm{dt} = \frac{w_i w_j}{2V_{cell}^2} \langle \sigma v \rangle_{ij} \mathrm{dt}$$

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$$N_{select} = f N_p$$

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Fractional-NTC Collisions:

- Select f by Cost/Accuracy Tradeoff
- Collision Δw Scaled for Skipped

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$$\Delta w_{ij} = \frac{N_p^2/2}{N_{select}} Z_{ij}$$

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Fractional-NTC Collisions:

- Select f by Cost/Accuracy Tradeoff
- Collision Δw Scaled for Skipped
- Add Particles & Original Reduced

$$Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle_{ij} \mathrm{dt} = \frac{w_i w_j}{2V_{cell}^2} \langle \sigma v \rangle_{ij} \mathrm{dt}$$

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$$N_{select} = f N_p$$
$$\Delta w_{ij} = \frac{N_p^2/2}{N_{select}} Z_{ij}$$
$$w_i{=}w_i - \Delta w_{ij} \ \& \ w_j{=}w_j - \Delta w_{ij}$$
$$w_{(N_p+1)}{=}\Delta w_{ij} \ \& \ w_{(N_p+2)}{=}\Delta w_{ij}$$

Review of Fractional Collisions

NTC Collisions:

- (Collision Rate Volume):(Cell Volume)
- Select Fraction of $\frac{1}{2}N^2$ Possible
- Probability of Event Ratio of Volumes
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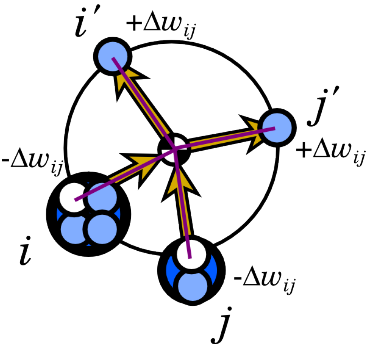
Fractional-NTC Collisions:

- Select f by Cost/Accuracy Tradeoff
- Collision Δw Scaled for Skipped
- Add Particles & Original Reduced
- +2 Particles/Collision! $\rightarrow$ Must Merge

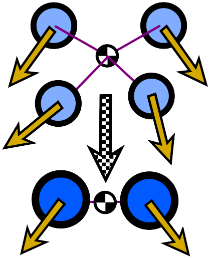
$$Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle_{ij} \,\mathrm{dt} = \frac{w_i w_j}{2V_{cell}^2} \langle \sigma v \rangle_{ij} \,\mathrm{dt}$$



$$w_i = w_i - \Delta w_{ij} \;\&\; w_j = w_j - \Delta w_{ij}$$
$$w_{(N_p+1)} = \Delta w_{ij} \;\&\; w_{(N_p+2)} = \Delta w_{ij}$$

Merge to Pair → DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF



$$w_{cell} = \sum_i^{(n+2)} w_i$$
$$\overline{\vec{v}} = \frac{1}{w_{cell}} \sum_i^{(n+2)} w_i \vec{v}_i$$
$$\overline{V^2} = \frac{1}{w_{cell}} \sum_i^{(n+2)} w_i \left(\vec{v}_i - \overline{\vec{v}}\right)^2$$

$$w_{(a/b)} = w_m/2$$
$$\vec{v}_{(a/b)} = \overline{\vec{v}} \pm \hat{\mathcal{R}}\sqrt{\overline{V^2}}$$

Similarly: $\vec{x}_{(a/b)} = \overline{\vec{x}} \pm \hat{\mathcal{R}}\sqrt{\overline{X^2}}$

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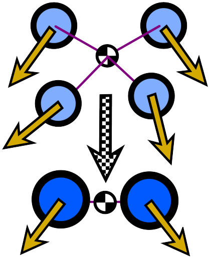
Selection of Near Neighbors in VDF Limits Thermalization

(≈ Near Neighbor Pairs in 2:1 Merges that Limit Numerical Cooling)



$$w_{cell} = \sum_i^{(n+2)} w_i$$
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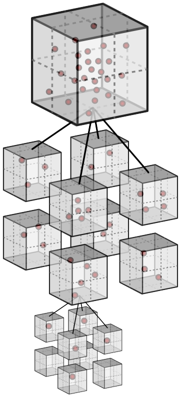
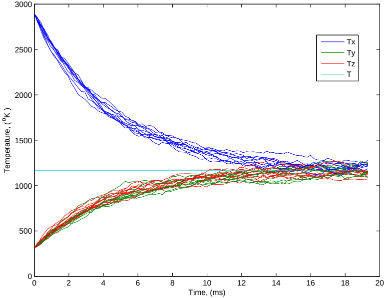
Octree Velocity Bins



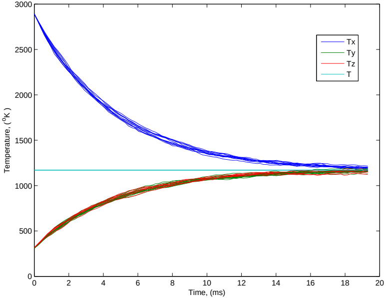
Efficient Neighbor Selection

Bi-Maxwellian Thermalization Results

Original-NTC



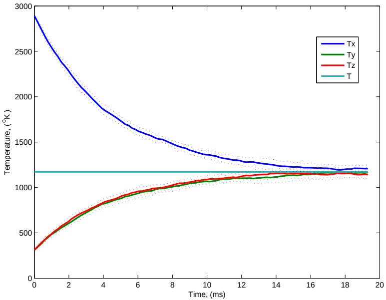
Fractional-NTC



Comparison of 10x Runs from Same Initial Distribution

Bi-Maxwellian Thermalization Results

Original-NTC



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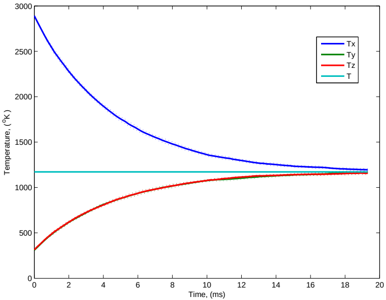
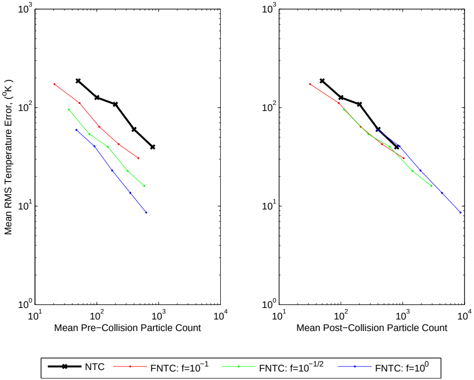


Mean and RMS Fluctuation of Sample Runs

Fluctuations Level Tuneable with f Independent of Particles Count

Bi-Maxwellian Thermalization Results



Fluctuations Level Tuneable with f Independent of Particles Count

- Initial Bi-Maxwellian Distribution in Potential Well

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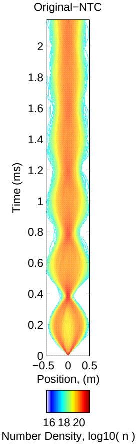
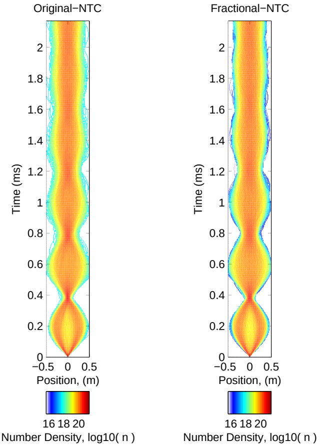
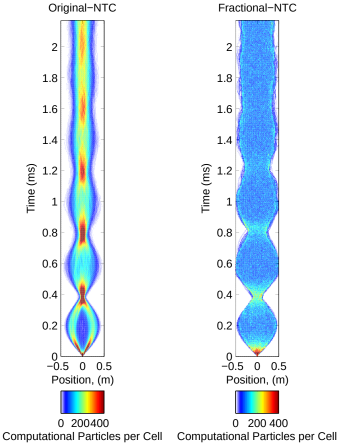
- NTC Collisions Results in Beam Thermalization



- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior



- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior
- Particles/Cell Dramatically Different



- Initial Bi-Maxwellian Distribution in Potential Well
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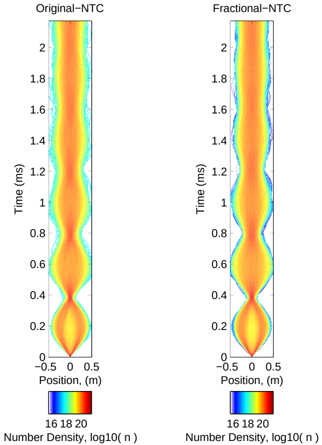
- Fractional-NTC Collisions Produce Same Behavior
- Particles/Cell Dramatically Different
- Fringe Extends to Lower Densities with Variable Weights



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- Particles/Cell Dramatically Different
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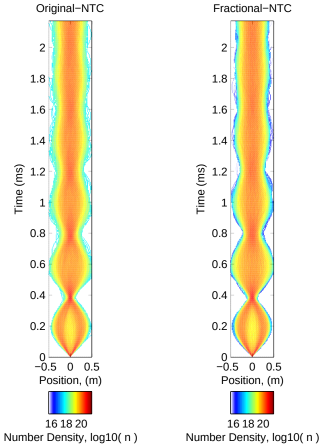
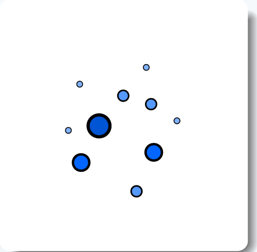
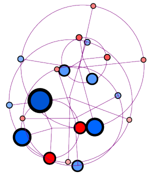
- Relative 'Error' Unknown without Analytical Solution or High Fidelity Simulation



- Larger $N_{select} \rightarrow$ Better Approx. of Collision Integral



- Larger $N_{select} \rightarrow$ Better Approx. of Collision Integral
- f-NTC Produces 2x-Particles per $N_{select} = f\ N_p$
- Particle Memory Requires $\propto\ N_{max} \rightarrow (1+2f)N_{max}$



- Larger $N_{select} \rightarrow$ Better Approx. of Collision Integral
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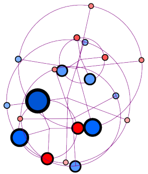

Issue with Collide then Merge

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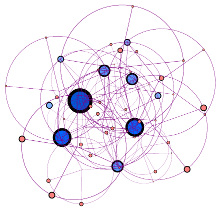

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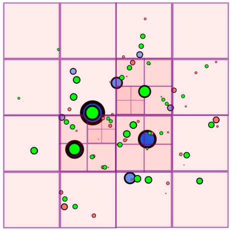
- Merge Immediately after Collide per Spatial Cell?..
- Sort for Merge still $\propto (1+2f)\ log(1+2f)$?



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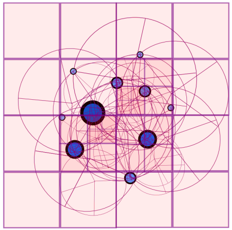
- Sort for Merge still $\propto (1+2f)\ log(1+2f)$?
- Combine Collision and Merge in Single Step?



- Fractional Collision as Rate Equation

$$\begin{bmatrix} \vdots \\ \dot{w}_i \\ \vdots \\ \dot{w}_j \\ \vdots \\ \dot{w}_{i'} \\ \vdots \\ \dot{w}_{j'} \\ \vdots \end{bmatrix} = \sum_{k=1}^{N_{select}} \begin{bmatrix} \vdots \\ -w_i \left\langle \sigma v \right\rangle_{ij}^{k} w_j \\ \vdots \\ -w_i \left\langle \sigma v \right\rangle_{ij}^{k} w_j \\ \vdots \\ w_i \left\langle \sigma v \right\rangle_{ij}^{k} w_j \\ \vdots \\ w_i \left\langle \sigma v \right\rangle_{ij}^{k} w_j \\ \vdots \end{bmatrix}$$

- Fractional Collision as Rate Equation
- Bin Moments needed for Particle Pairs

$$\begin{bmatrix} \dot{w}_i \\ \dot{w}_j \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ - \\ (\dot{wv})_i \\ (\dot{wv})_j \\ (\dot{wv})_{i'} \\ (\dot{wv})_{j'} \\ - \\ (\dot{wv^2})_i \\ (\dot{wv^2})_j \\ (\dot{wv^2})_{i'} \\ (\dot{wv^2})_{j'} \end{bmatrix} = \sum_{k=1}^{N_{select}} \begin{bmatrix} -\Delta w_{ij} \\ -\Delta w_{ij} \\ \Delta w_{ij} \\ \Delta w_{ij} \\ - \\ -\Delta w_{ij} v_i \\ -\Delta w_{ij} v_j \\ \Delta w_{ij} v_{i'} \\ \Delta w_{ij} v_{j'} \\ - \\ -\Delta w_{ij} v_i^2 \\ -\Delta w_{ij} v_j^2 \\ \Delta w_{ij} v_{i'}^2 \\ \Delta w_{ij} v_{j'}^2 \end{bmatrix}$$

- Fractional Collision as Rate Equation
- Bin Moments needed for Particle Pairs
- Particle Pairs (i,j) Picked Randomly
- DSMC-like Collision (VHS,VSS,etc.)
  Random $\chi, \theta \rightarrow (v_{i'}, v_{j'})$

$$
\begin{bmatrix}
\dot{w}_i \\ \dot{w}_j \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ - \\ (\dot{wv})_i \\ (\dot{wv})_j \\ (\dot{wv})_{i'} \\ (\dot{wv})_{j'} \\ - \\ (\dot{wv^2})_i \\ (\dot{wv^2})_j \\ (\dot{wv^2})_{i'} \\ (\dot{wv^2})_{j'}
\end{bmatrix}
= \sum_{k=1}^{N_{select}}
\begin{bmatrix}
-\Delta w_{ij} \\ -\Delta w_{ij} \\ \Delta w_{ij} \\ \Delta w_{ij} \\ - \\ -\Delta w_{ij} v_i \\ -\Delta w_{ij} v_j \\ \Delta w_{ij} v_{i'} \\ \Delta w_{ij} v_{j'} \\ - \\ -\Delta w_{ij} v_i^2 \\ -\Delta w_{ij} v_j^2 \\ \Delta w_{ij} v_{i'}^2 \\ \Delta w_{ij} v_{j'}^2
\end{bmatrix}
$$

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- DSMC-like Collision (VHS,VSS,etc.)
  Random $\chi, \theta \rightarrow (v_{i'}, v_{j'})$
- Octree to Find i' and j' Bins
  $8^L \rightarrow$ Few Levels to Search

$$
\begin{bmatrix} \dot{w}_i \\ \dot{w}_j \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ - \\ \dot{(wv)}_i \\ \dot{(wv)}_j \\ \dot{(wv)}_{i'} \\ \dot{(wv)}_{j'} \\ - \\ \dot{(wv^2)}_i \\ \dot{(wv^2)}_j \\ \dot{(wv^2)}_{i'} \\ \dot{(wv^2)}_{j'} \end{bmatrix} = \sum_{k=1}^{N_{select}} \begin{bmatrix} -\Delta w_{ij} \\ -\Delta w_{ij} \\ \Delta w_{ij} \\ \Delta w_{ij} \\ - \\ -\Delta w_{ij} v_i \\ -\Delta w_{ij} v_j \\ \Delta w_{ij} v_{i'} \\ \Delta w_{ij} v_{j'} \\ - \\ -\Delta w_{ij} v_i^2 \\ -\Delta w_{ij} v_j^2 \\ \Delta w_{ij} v_{i'}^2 \\ \Delta w_{ij} v_{j'}^2 \end{bmatrix}
$$

- Fractional Collision as Rate Equation
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Conserve Mass, Momentum, and Energy
Memory Constant Independent of N^{select}

$$
\begin{bmatrix} \dot{w}_i \\ \dot{w}_j \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ - \\ \dot{(wv)}_i \\ \dot{(wv)}_j \\ \dot{(wv)}_{i'} \\ \dot{(wv)}_{j'} \\ - \\ \dot{(wv^2)}_i \\ \dot{(wv^2)}_j \\ \dot{(wv^2)}_{i'} \\ \dot{(wv^2)}_{j'} \end{bmatrix} = \sum_{k=1}^{N_{select}} \begin{bmatrix} -\Delta w_{ij} \\ -\Delta w_{ij} \\ \Delta w_{ij} \\ \Delta w_{ij} \\ - \\ -\Delta w_{ij} v_i \\ -\Delta w_{ij} v_j \\ \Delta w_{ij} v_{i'} \\ \Delta w_{ij} v_{j'} \\ - \\ -\Delta w_{ij} v_i^2 \\ -\Delta w_{ij} v_j^2 \\ \Delta w_{ij} v_{i'}^2 \\ \Delta w_{ij} v_{j'}^2 \end{bmatrix}
$$

Non-linear Equation in Terms of Weights:

$$\frac{\delta Q}{\delta t} = F(Q)$$

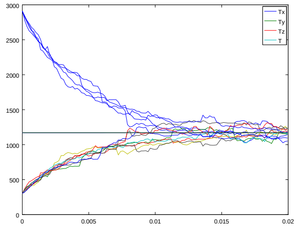
Amenable to Time Marching Schemes?

Non-linear Equation in Terms of Weights:

$$\frac{\delta Q}{\delta t} = F(Q)$$

Explicit:

$$\delta Q = \Delta t F(Q)$$



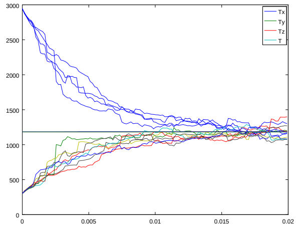
Non-linear Equation in Terms of Weights:

$$\frac{\delta Q}{\delta t} = F(Q)$$

Predictor Corrector:

$$\overline{\delta Q} = \frac{\Delta t}{2}\left(F(Q^0) + F(Q^0 + \delta Q)\right)$$

(Iterate for δQ ?)



Non-linear Equation in Terms of Weights:

$$\frac{\delta Q}{\delta t} = F(Q)$$

Linearized Crank-Nicolson:

$$\delta Q = \Delta t \left(F(Q^0) + \frac{1}{2} \left. \frac{\delta F}{\delta Q} \right|^0 \delta Q \right)$$

$$\delta Q = \Delta t \left(I - \frac{\Delta t}{2} \left. \frac{\delta F}{\delta Q} \right|^0 \right)^{-1} F(Q^0)$$

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$$\frac{\delta Q}{\delta t} = F(Q)$$

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But Complex in v_i, v_j in Terms of Q...

Non-linear Equation in Terms of Weights:

$$\frac{\delta Q}{\delta t} = F(Q)$$

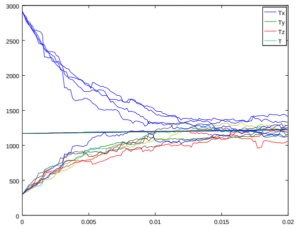
Linearized Crank-Nicholson:

$$\delta Q^{(w)} = \Delta t \left(F(Q^{(w),0}) + \frac{1}{2} \left. \frac{\delta F^{(w)}}{\delta Q^{(w)}} \right|^{0} \delta Q^{(w)} \right)$$

$$\delta Q^{(w)} = \Delta t \left(I - \frac{\Delta t}{2} \left. \frac{\delta F^{(w)}}{\delta Q^{(w)}} \right|^{0} \right)^{-1} F(Q^{(w),0})$$

$$\delta Q^{(M)} \approx \Delta t \left(F(Q^{(M),0}) + \frac{1}{2} \left. \frac{\delta F^{(M)}}{\delta Q^{(w)}} \right|^{0} \delta Q^{(w)} \right)$$

But Complex in v_i, v_j in Terms of Q...
First Assume Primary Dependance on δw..?



Marching Worse than Original F-NTC?

$$\frac{\delta Q}{\delta t} = F(Q)$$

Approximation of Random Discrete Jump Process

DIRECT TIME MARCHING?

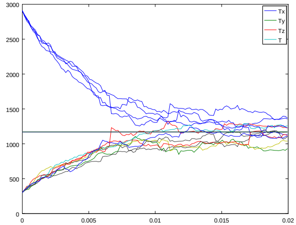
Marching Worse than Original F-NTC?

$$\frac{\delta Q}{\delta t} = F(Q)$$

Continuous:

$$\delta Q \approx \Delta t F(Q) \rightarrow \delta Q = \int_0^{\Delta t} F(Q(t))dt$$

Order of Jumps is Random
Approximates Nature as $N^{select} \rightarrow \infty$ Increase
$f \rightarrow$ Smaller Jumps Indpendent of Δt
Continuous Update of Q$\approx$ VDF Evolution



Conclusion

- Standard Collision Incompatible with Variable Weight
- Fractional-NTC Option for Variable Weight Collision
- Bin-To-Bin F-NTC Potentially Alleviates Memory Constraints
- Bin-To-Bin also Allows Route to Advanced Time Marching
- Preliminary Advanced Time Marching Requires Additional Study
- Verification vs. Standard Shock Cases/etc. Needed

Thank You

Questions?